Clarification of the Bootstrap Percolation Paradox

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We study the onset of the bootstrap percolation transition as a model of generalized dynamical arrest. We develop a new importance-sampling procedure in simulation, based on rare events around "holes", that enables us to access bootstrap lengths beyond those previously studied. By framing a new theory in terms of paths or processes that lead to emptying of the lattice we are able to develop systematic corrections to the existing theory, and compare them to simulations. Thereby, for the first time in the literature, it is possible to obtain credible comparisons between theory and simulation in the accessible density range.

The bootstrap percolation [1, 2] problem has attracted considerable interest from a variety of scientific communities. In essence it (or its obvious variants) is a method to analyze the dynamics of a system of highly coupled units, each of which has a state that depends on those of its close neighbors. Such units have been considered particles, processors, or elements of a growing population. Units that become active in the underlying dynamics are simply removed in the bootstrap. The ensemble can undergo a transition to an "arrested" state in which all dynamics is quenched, and this is (after bootstrap removal of units) reflected in a transition from an empty to partially filled lattice. This arrest is found to be driven by a long length scale. The change of state of one unit becomes increasingly difficult near arrest, requiring a long sequential string of favorable changes in its surrounding units. Thereby a long length (the size of the surrounding region to be changed) is slaved to a long (relaxational) time scale.

The simplicity of bootstrap concepts means that bootstrap percolation plays a canonical role in the conceptual framework of the dynamical arrest transition, "classification" [3, 4, 5] and in arenas as diverse as processor arrays [6] and crack propagation [7] amongst others.

We study two types of "dynamics", the well-known "bootstrap model" itself [1, 8, 9, 10], and the modified bootstrap [7, 11]. In the former, particles are removed if they are surrounded by c or less neighbors, and in the latter they are removed if any two of its vacant nearest neighbors are also second neighbors to each other. The (random bootstrap) transition occurs as a function of c, system size L, and initial particle density ρ and occurs when half of the prepared initial states are empty after removal of all movable particles.

In this paper we introduce both new simulation algorithms and theoretical approaches that qualitatively change the regimes that may be explored. The theory is now relevant to physically accessible length-scales and, using only a personal computer, the simulations can be extended beyond the largest scales currently accessible in the most advanced simulations. A most interesting outcome, perhaps of topical interest [12], is that we are able to elucidate the origin of disagreements between simu-

lation [7, 13] and theory [14, 15, 16] for the bootstrap models, and show how the two can work together more closely in future developments. Currently our calculations are detailed and specific to these models, but we consider they contain the kernel of generality required to signpost the path to future developments in the whole arena of dynamical arrest.

The bootstrap-type problems mentioned above fall into two broad "universality" classes of arrest transition [1]. The first type is a continuous or "critical" point transition in which progressively more particles lose motion, leading to growing arrested domains whose typical size diverges with a power law. The second type of transition (of interest to us here), is more reminiscent of a first-order transition. There, dynamically slowed domains grow near arrest according to an essential singularity. Mobilization of these domains is dependent on rare events (we call these "connected holes" [17]) involving specific units that can nucleate motion on this large length. As will become clear, these nuclei become highly dilute near the transition, the typical distance between them being the diverging bootstrap length.

For such transitions the following conclusions have been drawn by the community. For $c = d$ (the dimension) it is believed that the bootstrap length ξ diverges according to an essential singularity $\xi^d = \exp^{\circ(d)}(-A/(1-\rho))$ where $\exp^{\circ(d)}$ is the exponential function iterated d times [1, 18]. For the two dimensional square lattice $c = 2$, theoretical calculations [15] have resulted in an elegant outcome; essentially what are believed to be exact results, $\lim_{\substack{\rho \to 1 \\ \xi \to \infty}} 2(1-\rho)\log\xi = A$, where $A = \pi^2/9$ and $\pi^2/3$ for conventional and modified bootstrap respectively.

On the other hand, all attempts to obtain this asymptotic result by simulation have so far failed, including extensive calculations up to $L = 128,000$, leading to speculation that it may be relevant to particle densities very close to unity, and consequently system sizes that are incredibly large (eg. $\xi \sim 10^{47}$ at $\rho = 0.995$ [19]). Such lengths would be far beyond what will ever be possible, or indeed of interest, for Physics to explore.

Buried within this problem, however, a more troubling implication emerges [2, 12, 15] that simulations and theory seem relevant to such different scales that there can

be little useful dialogue between them. The point is also well made that many of the interesting arenas of application involve large, but finite number of units, and the present theory does not seem helpful there [2]. We will show that this need not be the case. When the problem is properly placed in context of general knowledge in the Physics community, the previous theory is useful, elegant and worth developing further, and the simulations were correct, and worthwhile.

We will show that the modified theory and simulation can be brought into agreement over all reasonable length scales of interest to Physics. Our results are exact also in the true asymptotic regime [15] but simulations cannot reach there and Physics will likely not be interested in the outcome. We identify "holes" on the lattice as spaces (vacancies) into which particles can move [17]. We then identify these holes as either "connected" or caged (disconnected) according to whether the lattice can (or cannot) be vacated by sequentially removing particles beginning from that hole. The relationship to conventional (random) bootstrap simulations (described above) is clear; a given system size and density must contain at least one connected hole for it to be vacated by random bootstrapping processes. Thus, the bootstrap correlation length ξ is related to the connected hole density ν via $\nu = 1/\xi^2$. The bootstrap length is therefore the average distance between connected holes (these representing the growth "nuclei" alluded to in our introductory remarks) that become increasingly rare near arrest. The device of holes allows us to focus on the key "order" parameter, rather than the very populous, but irrelevant particles and vacancies [17].
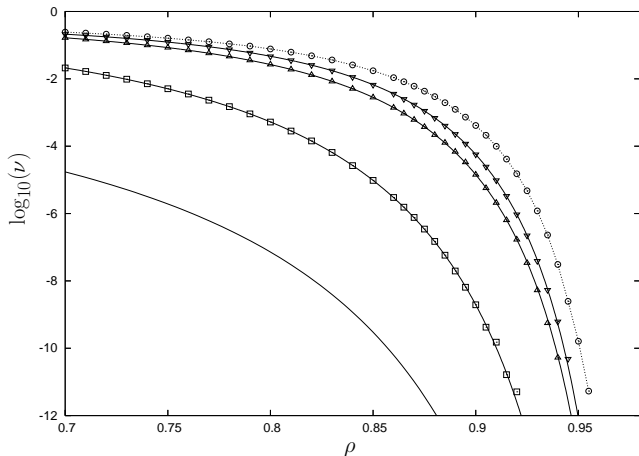
The details will be presented elsewhere, so here we present only some results for the case $d = 2$. In the simulations we begin by creating a hole with the appropriate weight, and then populate ('grow') the configuration with particles and vacancies around this site, checking at each stage to see if that hole is connected, or trapped (ie a rattler [17]) by identifying cages at that length. Since the typical cage size grows much more slowly $(\log(1-\rho)/\log(\rho))$ than the bootstrap length, we need check only relatively small distances before the transition probability of bootstrap to the next largest length approaches unity, and the hole is connected with certainty. This approach has significant practical advantages since it permits us to sample directly only the important rare events (connected holes) rather than prepare and study very large systems. Thus, the results produced here require only a few hours of time on a personal computer. In Figure 1 and Figure 2 we show results for the total connected hole density in the modified and conventional bootstrap model, and these agree, where comparisons are available, with the most extensive conventional simulations. For example, the ($\diamond$) points in the uppermost curve of Figure 2) represent the hole density implied by the results in [2, 20] (system size $L = 128,000$), while the ($\circ$) points on that same curve are from our importance-sampling procedure discussed above. An additional advantage in the simulation approach is that we can make direct contact with theory.

Previous theoretical calculations [3, 11, 15] approximate the process of simultaneous removal of particles on increasingly large boundary contours until reaching one that is entirely occupied by particles, and therefore
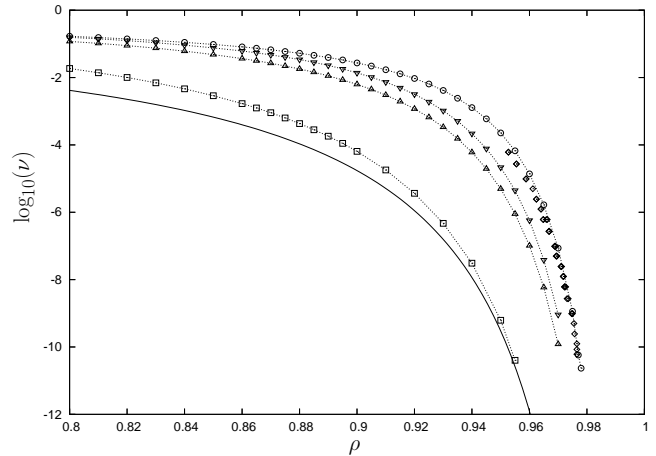

FIG. 1: Modified Bootstrap Model. The ($\circ$) points represent the total hole density (the dotted line is a guide to the eye). The symmetrically growing squares ($\square$) are compared with the asymptotic result $\exp(-\pi^2/3(1-\rho))$ (lower solid line) [15]. Also shown are results for diffusing squares ($\triangle$) and small-asymmetry rectangles (∇)- in these cases, the lines through the points represent our theoretical results.

FIG. 2: Bootstrap Model. The ($\circ$) points represent the total hole density (the dotted line is a guide to the eye) and can be compared with the results for $1/\xi^2$ ($\diamond$) for $\xi > 100$ [2, 20]. The symmetrically growing squares ($\square$) are compared with the asymptotic result $\nu = \exp(-\pi^2/9(1-\rho))$ (lower solid line) [15]. Also shown are results for diffusing squares ($\triangle$) and small-asymmetry rectangles (∇).

immovable. The theory presented here is developed by finding the most important 'paths' or sequences by which particles are removed, counting the number of holes that would be connected using such a set of paths. Addition of new path types systematically improves the result, making comparison to theory feasible for the first time.

Schematically, the probability of bootstrap $\nu = P_\infty$ is represented $P_\infty = \Pi_{k=1}^\infty (1 - \rho^{ak})^b$, where b represents the number of sides and a the increment on the lattice. In the high density limit one takes the natural logarithm of the product, approximates the sum with an integral and makes the substitution $y = \rho^k$. For $\rho \to 1$ this leads to $-b/(a \ln \rho) \int_0^1 (dy/y) \ln(1-y) \sim -b\pi^2/6a(1-\rho)$ [19]. In the modified bootstrap model, $a = 2$ and $b = 4$, one obtains $-\pi^2/3(1-\rho)$, and it is this result that has been proven to be asymptotically exact [15]. From Figure 1 it is clear (as has often been reported) that there is no agreement between the simulated results for the total hole density ($\circ$) and the asymptotic result, even for the highest densities we can simulate. It is important to ask how much of this deviation comes from the limited set of paths included in the theory and how much from the fact that simulations can never reach the truly asymptotic limit. Thus, we calculate exactly the probability for removal of concentric squares of particles, a result that includes all corner contributions, and is valid for all densities. Then,

$$P_\infty^{(cs)} = (1-\rho)\Pi_{k=1}^\infty c_k^{(cs)}(\rho) \qquad (1)$$
$$c_k^{(cs)}(\rho) = 1 - 4\rho^{2k+1} + 2\rho^{4k+1}(2+\rho) - 4\rho^{6k+1} + \rho^{8k}$$

Using $(1 - \rho^{2k+1})^4$ as lower bounds for the coefficients $c_k^{(cs)}(\rho)$ and we find a modified asymptotic result for the hole density $(1-\rho)^{-5}\exp(-A/(1-\rho))$ [19]. This modified asymptotic result is almost equal to our numerical solution of Equation 2 and simulation results for the symmetrically growing squares process in the density range of interest. While these are in perfect agreement with each other (see ($\square$) in Figure 1), they are still many orders of magnitude different from the full simulated connected hole density, although there is clearly a considerable improvement over the purely asymptotic result $\exp(-\pi^2/3(1-\rho))$.

Nevertheless, by permitting only such restricted paths we have failed to correctly identify many holes as connected. Our aim now in development of the theory is therefore to systematically enlarge the possible paths in the calculation, until we approach the full simulated result, at each stage validating the theoretical calculation by simulating the same restricted set of paths. By simulation it is easy to show that indeed paths involving symmetric removal are the most probable, but the constraint that all particles be removed from the boundary in a single step results in loss of many holes. If instead the boundary particles are simultaneously removed only on adjacent sides of the square, then the emptying squares

are also permitted to "diffuse", that is, change their center of gravity during the process. This leads us to identify many new holes that would otherwise be wrongly identified as disconnected. One can go one stage further, and permit even asymmetric paths, eventually exhausting all paths. However, by binning the paths adopted in the simulation of the total connected hole density we find that throughout the whole emptying process, beginning from a connected hole, the ratio of the rectangular sides never exceeds 1.4, by far the greatest contribution coming from near-square process, providing they are permitted to diffuse. We have been able to realize this approximation in theory also. We define intermediate states of the system as the squares illustrated in Figure 3, with weight $P_k^{(i)}$. Paths implied by removal of particles map the growing vacant region between only these states, larger by one step at each stage. If we consider only the limited set P^1 - P^3, such processes correspond to growing and diffusing squares. Inclusion of the states P^4 and P^5 permits in addition "fluctuations" of the square by one additional layer. These local intermediate states are related by the coupled equations,

$$P_k^{(i)}(\rho) = \sum_j c_k^{(i,j)}(\rho) P_{k-1}^{(j)}(\rho) \qquad (2)$$

where i, j's range from $1 \to n$, with $n = 3$ in the diffusing squares process, and $n = 5$ in its extended small-asymmetric rectangular version. $c_k^{(i,j)}(\rho)$ defines the probability of migration from class j to i at the kth step. These equations are solved subject to the initial

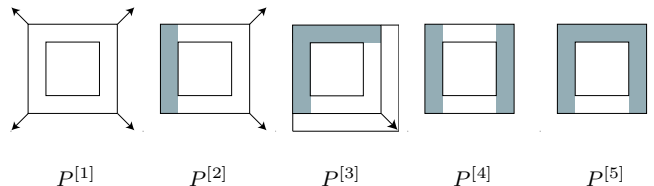$P^{[1]}$ $\qquad$ $P^{[2]}$ $\qquad$ $P^{[3]}$ $\qquad$ $P^{[4]}$ $\qquad$ $P^{[5]}$

FIG. 3: Intermediate configurations arising in evaluation of the sum over 'paths' that may be used to empty the lattice. The inner square from each of these figures is assumed to have been emptied of particles in the previous step, and the next parts to be emptied lie between this and the outer bounding square. Shaded outer regions imply a complete line of particles, blocking further movement in that direction. Unshaded outer regions have at least one vacancy in that part of the perimeter. The arrows on the squares indicate possible transitions involving the growth of two adjacent boundary lines by one step. This process restores that local configuration to one of the intermediate states again, with the internal empty square one step larger in two directions. The process terminates when the local configuration makes a transition outside of the class P^1 - P^3 (diffusing squares) or P^1 - P^5 for small-asymmetry rectangles. Note that in P^3 we have given an explicit example of the extension of the boundary implied by the arrow.

conditions, $P_1^{(i)} = (1-\rho)\delta_{1i}$.

The choice of these states, and transitions between them, is far from trivial since we must ensure an "ordering" of the removal process if we wish to use a random measure for the particles in calculating the coefficients $c_k^{(i,j)}(\rho)$. For the sake of simplicity, we here present only the coefficients of the process involving diffusing squares,

$$c_k^{(1,1)} = 1 - 2\rho^{2k} + \rho^{2k-1}, c_k^{(1,2)} = (1-\rho)(1-\rho^k)$$
$$c_k^{(1,3)} = (1-\rho)^2, \qquad c_k^{(2,1)} = 2\rho^k(1-\rho^{k-1})$$
$$c_k^{(2,2)} = 1 - 2\rho^k + \rho^{2k-2}, c_k^{(2,3)} = 2\rho(1-\rho-\rho^{k-1}+\rho^k)$$
$$c_k^{(3,1)} = \rho^{2k-1}, \qquad c_k^{(3,2)} = \rho^k(1-\rho^{k-1})$$
$$c_k^{(3,3)} = \rho^2(1 + 2\rho^{k-2} - 4\rho^{k-1} + \rho^{2k-3})$$

The total bootstrap probability $P_\infty^{(1)}(\rho)$, may be calculated numerically for any density, limited only by the precision of the computer. The same processes may be simulated on the computer and are in each case identical with the theory. Results for all are given in Figure 1 and Figure 2 for modified and conventional bootstrap.

The outcome is intriguing. Diffusing squares ($\triangle$), improves the comparison between theory and full simulation, and small-asymmetry rectangles ($\triangledown$) yields results that may (for the first time) begin to be credibly compared to computer simulation of the full simulated hole density, and implicitly the bootstrap correlation length in the regime where simulations can be carried out.

We may now summarize our results both in relation to the bootstrap problem, and in a more broad context. Firstly, for the bootstrap problem itself, new computational and theoretical approaches have enabled simulations and theory to be brought into reasonable (indeed arbitrarily good) agreement across a wide range of density. The fact is that both the theory and simulation do not adopt the very simple asymptotic form that has been quoted in the literature until one reaches densities and length scales that are beyond the natural interest of physics. There nevertheless remain many areas of physics where extended regimes of dynamic slowing, and near-arrest are of great importance, and these can be dealt with by the methods described here. Secondly, by properly identifying the most probable paths (incidently thereby respecting the symmetry of the problem), and developing theory as a sum over only these paths, we obtain a very useful approximation, and systematic corrections around it. In essence this amounts to a sort of "mean-field" approximation in the path-integral (sum), more familiar in field theory as the optimal instanton trajectory [21]. Inclusion of small asymmetry is equivalent to the 'shape' fluctuations included in next to leading order in such calculations. This is more than an analogy; the bootstrap process of this discontinuous transition produces an essential singularity precisely because,

underlying it, is the physics of complex activated processes.

In this second point, but from a broader perspective, we have linked the whole bootstrap endeavor (and crucially those areas of physics for which it is considered relevant) to an arena of physics that is already somewhat explored, and opened the pathway to numerous developments in the theory of dynamical arrest, many of which will immediately suggest themselves to the reader.

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